

## ON-LINE DIAGNOSIS OF ABNORMAL SITUATIONS IN AN INDUSTRIAL STYRENE POLYMERIZATION REACTOR

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### ABSTRACT

This paper deals with the robust on-line diagnosis of abnormal situations in an industrial continuous styrene polymerization reactor through a bank of unknown input observers (UIO) that supervise changes on the most relevant process parameters and external disturbances. A model predictive control (MPC) scheme is implemented aiming at to stabilize the system. This may become an additional difficulty because the detrimental effects of the feedback control on the detection of abnormal situations. In the design of the UIO's a linearized model of the process is utilized. The observers are tuned to supervise the change of a particular parameter of the reactor model. The procedure takes into account possible uncertainties in these parameters such that a robust diagnosis strategy of the abnormal situation is obtained. Simulation results show a very promising perspective to the proposed strategy.

**Keywords:** Fault Diagnosis, Abnormal Situation Management, Unknown Input Observers, Model Predictive Control, Polymerization Reactors.

### 1. INTRODUCTION

Over the last 20 years, industrial companies have invested to improve process operations by introducing Process Systems Engineering (PSE) techniques, such as advanced control systems, namely Model Predictive Control (MPC), and Real Time Optimization (RTO). In many cases these investments have led to impressive returns on investment, with payback times measured in weeks or months. While these investments will continue, today, industrial companies are seeking to address the impact of abnormal situations.

Abnormal situation is a general term used to describe any significant disturbance that drives the process to an operating point far from its acceptable range of operation, and where the control system cannot efficiently deal with disturbances. In this circumstance, and in order to achieve effective correction abnormal situation, an operator has to perform a

complex sequence of decision tasks as detection of abnormalities, identification of the root causes of faults and magnitudes, and planning of corrective actions. However, in a real-life plant environment, these tasks are not very easy, mainly because the scale and complexity of modern plants and overload or even contradictory flow of information, that an operator must deal with. As a result, wrong decisions are taken which lead to premature plant shutdowns, sub-optimal operation of the process and violations of safety and environmental rules. Industrial statistics pointed that between 40% and 80% of accidents in chemical process industries are caused by operator errors (Sebzali and Wang, 2002). In addition, the demand by increased productivity which forces the processes to operate in critical conditions, increasing the possibility of system failures that can potentially result in plant breakdown, with loss of productivity, loss of expensive equipment

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and, ultimately, human lives (Huang et al., 2002). To tackle these problems, lessons from the aviation are being transferred to industrial processes to achieve higher performance, efficiency, reliability and safety. To reach these goals, it is necessary to supervise the production process, i.e. to diagnose faults while the plant is still operating in a controllable region, to support operator to deal with abnormal situations promptly. In this sense, fault diagnosis (FD), i.e. fault detection, fault isolation and fault estimation can be seen as part of a large scheme for optimal process operation.

The proper operation of the industrial polymerization reactor is a significant business opportunity for PSE applications, which is commonly called polymerization reactor engineering in a broad sense, obstructed by multiple technical and practical challenges. The technical challenges are specific to the particular case, but they are generally due to their intrinsic characteristics such as nonlinearity, multivariable and interactive dynamic behavior, potential open-loop instability and multiple steady-states, highly exothermic reactions, varying process conditions, unknown reaction kinetics and high viscosity. The practical challenges are often more significant than the technical ones. The operation solution must be sustainable over the long term and robust to abnormal situations. These challenges are re-forced by the difficulty to detect what is occurring inside the reactor at a given instant, and how the properties of the polymer are evolving as a function of time. Moreover, it can be difficult to identify whether or not the information coming from the process is reliable without adapted tools. Furthermore, in the case that the process is not performing as it should, it can be very difficult to tell which component is responsible for the abnormality. Thus the difficulty of monitoring polymerization on-line and the impossibility of post-synthesis purification make proper fault detection techniques so useful (Kaboré et al., 2000).

Although there are a quite large number of studies on polymerization reactor engineering, they are mainly dedicated to such aspects as

designing, modeling, simulation, optimization and control (Embiruçu et al., 1996). Very few studies have been focused on FD. Among these few works, Kaboré et al. (2000) use non-linear high-gain observers, Tatara and Cinar (2002) use knowledge-based systems and Kumar et al. (2003) use statistical approaches. In this paper, linear observers are used in the design of a robust FD system for on-line diagnosis of abnormal situations in a styrene polymerization process. First of all, a MPC control strategy is implemented aiming at to stabilize the system. Next a bank of Unknown Input Observers (UIO's) is used for fault detection of the most relevant process parameters and external disturbances; meanwhile a structured residual approach is used for fault isolation. Finally, estimation of the fault magnitude is performed using the freedom remaining in the observer design. The design of the UIO's is based on a linearized model of the process. The effectiveness of the proposed strategy is verified through numerical simulations carried out on an industrial styrene polymerization reactor.

## II. THE POLYMERIZATION REACTOR

The polymerization reactor is usually the heart of the polymer production process. In this paper, the industrial process described by Maner et al. (1996), for free-radical initiated bulk and solution styrene polymerization in a jacketed continuous stirred tank reactor (CSTR) is used. A simplified schematic diagram of this process is shown in Figure 1.

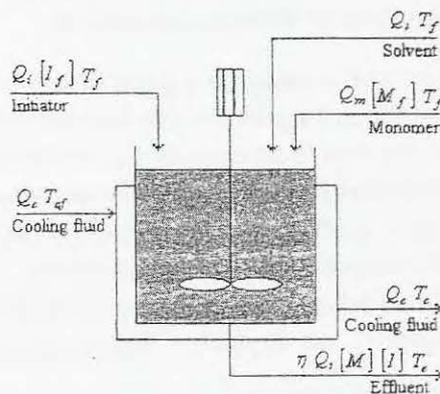


Figura N.º 1. Schematic diagram of the styrene polymerization reactor.

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$$\frac{d[U]}{dt} = \dots$$

$$\frac{d[M]}{dt} = \dots$$

$$\frac{d[T_c]}{dt} = \dots$$

$$\frac{d[T_c]}{dt} = \dots$$

$$\frac{dD_c}{dt} = 0.$$

$$\frac{dD_1}{dt} = M$$

$$\eta = 0.001$$

where

$$M_w =$$

$$k_j = A$$

$$j = i, P$$

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The CSTR has three feed streams: pure styrene monomer, azobisisobutyronitrile (AIBN) initiator dissolved in benzene and pure benzene solvent. Assuming the standard mechanism for free-radical polymerization, the following model for this polymerization process from Maher et al. (1996) is presented:

$$\frac{d[I]}{dt} = \frac{(Q_i[I_f] - Q_i[I])}{V} - k_i[I] \quad (1)$$

$$\frac{d[M]}{dt} = \frac{(Q_m[M_f] - Q_i[M])}{V} - k_p[M][P] \quad (2)$$

$$\frac{d[T_e]}{dt} = \frac{Q_i(T_f - T_e)}{V} + \frac{(-\Delta H_r)k_p[M][P]}{\rho C_p} - \frac{hA}{\rho C_p V}(T_e - T_c) \quad (3)$$

$$\frac{d[T_c]}{dt} = \frac{Q_c(T_{cf} - T_c)}{V_c} + \frac{hA}{\rho_c C_{pc} V_c}(T_e - T_c) \quad (4)$$

$$\frac{dD_0}{dt} = 0.5k_t[P]^2 - \frac{Q_i D_0}{V} \quad (5)$$

$$\frac{dD_1}{dt} = M_w k_p[M][P] - \frac{Q_i D_1}{V} \quad (6)$$

$$\eta = 0.0012(M_w)^{0.71} \quad (7)$$

where

$$M_w = \frac{D_1}{D_0}; [P] = \left[ \frac{2f_i k_i [I]}{k_t} \right]^{0.5};$$

$$k_j = A_j \exp\left(\frac{-E_j}{T_e}\right)$$

$$j = i, p, t$$

$$Q_t = Q_i + Q_s + Q_m$$

Equation (7) is included in the model to simulate measurements of the intrinsic viscosity ( $\eta$ ) instead of the number average molecular weight ( $M_w$ ), which is rarely available on-line. The process has three steady-states, but it is designed to operate in the middle point, because of the high conversion it provides. Process parameters and steady-state operational conditions are listed in Tables 1 and 2, respectively. For more details about the model, the interested reader is referred to the original reference.

Table N° 1. Process parameters for the polymerization reactor.

Variable description	Tag	Value
Frequency factor in Arrhenius equation for initiation reaction	$A_i$	$2.142 \times 10^{17}$ 1/h
Activation energy for initiation reaction	$E_i$	14,897 °K
Frequency factor in Arrhenius equation for propagation reaction	$A_p$	$3.816 \times 10^{16}$ L/(mol h)
Activation energy for propagation reaction	$E_p$	3557 °K
Frequency factor in Arrhenius equation for termination reaction	$A_t$	$4.5 \times 10^{12}$ L/(mol h)
Activation energy for termination reaction	$E_t$	843 °K
Initiator efficiency	$f_i$	0.6
Heat of polymerization reaction	$-\Delta H_r$	16,700 cal/mol
Monomer molecular weight	$M_m$	104.14 g/mol
Overall heat transfer coefficient x Heat transfer area of CSTR	$hA$	$2.52 \times 10^5$ cal/(°K h)
Mean density of reactor fluid x Mean heat capacity of reactor fluid	$\rho C_p$	360 cal/(°K L)
Density of cooling jacket fluid x Heat capacity of cooling jacket fluid	$\rho_c C_{pc}$	966.3 cal/(°K L)

Table N° 2. Steady-state operational condition for the polymerization reactor.

Variable description	Tag	Value
Flowrate of solvent	$Q_s$	459 L/h
Flowrate of monomer	$Q_m$	378 L/h
Reactor volume	$V$	3000 L
Volume of cooling jacket	$V_c$	3312.4 L
Temperature of reactor feed	$T_f$	330 °K
Inlet temperature of cooling jacket fluid	$T_{cf}$	295 °K
Concentration of initiator in feed	$[I_f]$	0.5886 mol/L
Concentration of monomer in feed	$[M_f]$	8.6981 mol/L
Concentration of initiator in reactor	$[I]$	$6.6832 \times 10^{-2}$ mol/L
Concentration of monomer in reactor	$[M]$	3.3245 mol/L
Temperature of cooling jacket fluid	$T_c$	305.17 °K
Molar concentration of the dead polymer chains	$D_0$	$2.7547 \times 10^{-4}$ mol/L
Mass concentration of the dead polymer chains	$D_1$	16.110 g/L
Flowrate of initiator	$Q_i$	108 L/h
Flowrate of cooling jacket fluid	$Q_c$	471.6 L/h
Intrinsic viscosity	$\eta$	2.9091 L/g
Temperature of reactor	$T_e$	323.56 °K

### III. THE CONTROL SYSTEM

The difficulties in designing an effective control system for the polymerization reactor arise from their intrinsic characteristics. MPC technology maybe a good alternative to deal with these problems (Schnelle and Rollins,

optimization 36). Very few FD. Among 100) use non- and Cinar systems and approaches.

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### REACTOR

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$$\frac{Q_s T_f}{\text{Solvent}}$$

$$\frac{[M_f] T_f}{\text{Monomer}}$$

$$\frac{Q_c T_c}{\text{Cooling fluid}}$$

$$\frac{[I] T_f}{\text{Initiator}}$$

the styrene

1998; Qin and Badgwell, 2003). In the present case, the first goal is to stabilize the system. For this purpose, a control system is designed aiming at to manufacture a uniform polymer with a target  $M_w$ , while regulating  $T_e$  for both safety and economic considerations. The control policy is carried out by manipulating  $Q_i$  and  $Q_c$ . However, as mentioned earlier, on-line measurement of is rarely available and is used instead, characterizing an inferential control approach.

For this process, a 2x2 MIMO control system, based on the infinite-horizon MPC (IHMPC) algorithm, as presented by Rodrigues and Odloak (2003), is implemented. The controller design incorporates an input-output linear process model, which is obtained by step response test. Some parameters of the IHMPC controller are the sampling time  $h$  and the control horizon. Other tuning parameters are not shown here. In addition to the MPC control structure, and in order to maintain a nearly constant volume fraction of solvent in the reactor, a ratio control law is implemented as (Maner et al., 1996):

$$Q_s = 1.5Q_m - Q_i \tag{8}$$

#### IV. ROBUST FAULT DETECTION WITH UNKNOWN INPUT OBSERVERS

Observer-based approach has become the most popular and important method for model-based FD (Patton and Chen, 1997; Frank and Ding, 1997), especially within the automatic control community. This method is based on the concept of analytical redundancy, where the inconsistency between the estimated and actual output is used as a residual ( $r$ ) or fault indicator. Later, the residual is evaluated and a simple binary decision ( $S_r$ ) is performed aiming at to decide if the fault has occurred. Observer-based fault detection approaches make use of the disturbance decoupling principle, in which the residual is designed, in the ideal case, by decoupling the effects of faults from unknown inputs (disturbances, noises and modeling errors), or decoupling the

effects of faults from each other for the purpose of fault isolation. A way to achieve this is by using the so-called unknown input observers (UIO's) (Chen and Patton, 1999).

UIO's are a generalization of the Luenberger observer that with a slight modification is used to solve the robust fault detection problem, and is designated as unknown input fault detection observer (UIFDO). Several methods such as algebraic, geometric, inversion approach, generalized inverse, singular value decomposition (SVD), and the Kronecker canonical form techniques have been proposed to the design of the UIFDO. Here, we follow the SVD approach proposed by Hou and Müller (1994).

We assume that in the presence of faults, a process can be represented by a linear time-invariant (LTI) system as follows:

$$\begin{aligned} x(k+1) &= Ax(k) + Bu(k) + Ef(k) \\ y(k) &= Cx(k) \end{aligned} \tag{9}$$

where  $x \in \mathbb{R}^{n \times 1}$  is the state vector,  $u \in \mathbb{R}^{m \times 1}$  is the input vector,  $y \in \mathbb{R}^{l \times 1}$  is the output vector,  $f \in \mathbb{R}^{q \times 1}$  is the fault vector and  $k$  is discrete sampling instant.  $A \in \mathbb{R}^{n \times n}$  is the system matrix,  $B \in \mathbb{R}^{n \times m}$  is the input matrix,  $C \in \mathbb{R}^{l \times n}$  is the output matrix and  $E \in \mathbb{R}^{n \times q}$  is the fault distribution matrix, which is assumed to be known. For the purpose of fault isolation, the vector  $f$  is partitioned into  $f = [f_1 \ f_2]^T$ . The vector  $f_1$  contains the faults that will be insensitive for the fault detector and the vector  $f_2$  contains the faults that will be monitored from the process. Even, the matrix  $E$  is partitioned into  $E = [E_1 \ E_2]$ . Here, the objective is to decouple from other faults in Eq. (9). For this purpose, consider the non-singular transformation matrix, where is obtained from the SVD of, i.e. . Thus, applying the state transformation to Eq. (9) results:

$$E_1 = U_1 \begin{bmatrix} \Sigma_1 \\ 0 \end{bmatrix} V_1^T$$

Thus, applying the state transformation  $z = Tx$  to Eq. (9) results:

$$\begin{aligned} z(k+1) &= \text{TAT}^{-1}z(k) + \text{TB}u(k) + \text{TE}_1f_1(k) + \text{TE}_2f_2(k) \\ y(k) &= \text{CT}^{-1}z(k) \end{aligned} \quad (10)$$

Consider the following partitions:

$$z(k) = \begin{bmatrix} z_1(k) \\ z_2(k) \end{bmatrix}; \quad \text{TAT}^{-1} = \begin{bmatrix} \text{A}_{11} & \text{A}_{12} \\ \text{A}_{21} & \text{A}_{22} \end{bmatrix};$$

$$\text{TB} = \begin{bmatrix} \text{B}_1 \\ \text{B}_2 \end{bmatrix}; \quad \text{CT}^{-1} = \begin{bmatrix} \text{C}_1 & \text{C}_2 \end{bmatrix};$$

$$\text{TE}_1 = \begin{bmatrix} \text{E}_{11} \\ 0 \end{bmatrix}; \quad \text{TE}_2 = \begin{bmatrix} \text{E}_{21} \\ \text{E}_{22} \end{bmatrix}$$

The transformed system can be divided into two subsystems as follows:

$$z_1(k+1) = \text{A}_{11}z_1(k) + \text{A}_{12}z_2(k) + \text{B}_1u(k) + \text{E}_{11}f_1(k) + \text{E}_{21}f_2(k) \quad (11)$$

$$z_2(k+1) = \text{A}_{21}z_1(k) + \text{A}_{22}z_2(k) + \text{B}_2u(k) + \text{E}_{22}f_2(k) \quad (12)$$

$$y(k) = \text{C}_1z_1(k) + \text{C}_2z_2(k) \quad (13)$$

If  $\text{C}_1$  is of full rank,  $z_1(k)$  can be eliminated from Eq. (12) by substituting  $z_1(k)$  obtained in Eq. (13). Otherwise, if it is not of full rank, consider a non-singular transformation matrix,

$\text{T}_1 = \text{U}_2^T$  such that  $\text{U}_2$  is obtained from the

SVD of,  $\text{C}_1 = \text{U}_2 \begin{bmatrix} \Sigma_2 \\ 0 \end{bmatrix} \text{V}_2^T$  i.e. Applying the

output transformation  $y^* = \text{T}_1y$  to Eq. (13) results:

$$y^*(k) = \text{U}_2^T y(k) = \begin{bmatrix} \Sigma_2 \\ 0 \end{bmatrix} \text{V}_2^T z_1(k) + \text{U}_2^T \text{C}_2 z_2(k) \quad (14)$$

Consider now the partitions:

$$y^*(k) = \begin{bmatrix} y_1^*(k) \\ y_2^*(k) \end{bmatrix}; \quad \text{U}_2^T \text{C}_2 = \begin{bmatrix} \text{C}_{21} \\ \text{C}_{22} \end{bmatrix}$$

Then, Eq. (14) can be written as follows:

$$y_1^*(k) = \Sigma_2 \text{V}_2^T z_1(k) + \text{C}_{21} z_2(k) \quad (15)$$

$$y_2^*(k) = \text{C}_{22} z_2(k) \quad (16)$$

Next, substituting  $z_1(k)$  from Eq. (15) into Eq. (12), and applying a Luenberger observer in the resulting equation, a UIFDO is obtained of the form:

$$\begin{aligned} \hat{z}_2(k+1) &= \bar{\text{A}}_{22} \hat{z}_2(k) + \text{B}_2 u(k) + \text{A}_{21} (\Sigma_2 \text{V}_2^T) \\ &+ y_1^*(k) + \text{K} (y_2^*(k) - \text{C}_{22} \hat{z}_2(k)) \end{aligned} \quad (17)$$

$$r(k) = y_2^*(k) - \text{C}_{22} \hat{z}_2(k) \quad (18)$$

where  $\bar{\text{A}}_{22} = \text{A}_{22} - \text{A}_{21} (\Sigma_2 \text{V}_2^T)^+ \text{C}_{21}$ . Equation (18) represents the residual vector. The observer gain  $\text{K}$  in Eq. (17) can be computed by the usual pole placement approach. Notice that the order of the UIFDO is  $(n - n_f)$ , where  $n_f = \text{rank}(\text{E}_1)$ . The following theorem states the existence conditions for this UIFDO.

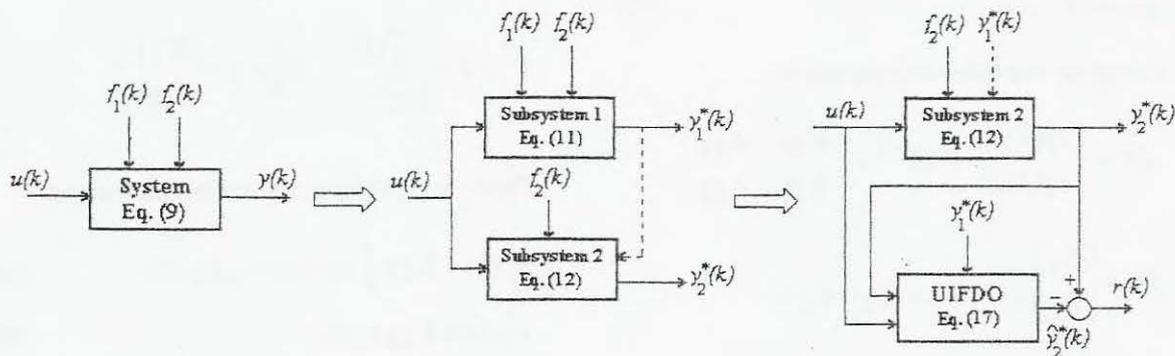
**Theorem:** Necessary and sufficient conditions for the existence of the UIFDO (Hour and Müller, 1994):

(i)  $\text{rank}(\text{CE}_1) = \text{rank}(\text{E}_1)$

(ii)  $(\text{C}_{22}, \bar{\text{A}}_{22})$  is a detectable pair.

The decoupling procedure of  $f_1$  from Eq. (9) and the structure of the UIFDO are illustrated in Figure 2.

Figure Nº 2. Fault decoupling procedure and structure of the UIFDO.

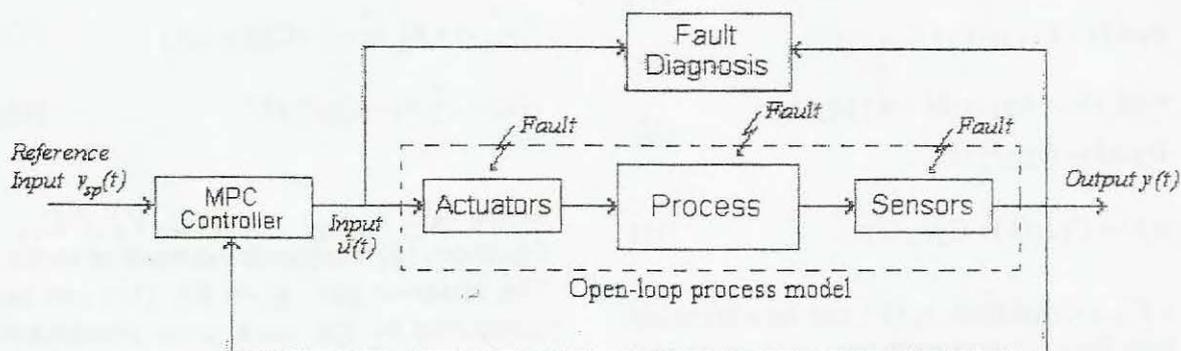


5. THE FAULT DIAGNOSIS SYSTEM

The FD system is based on an open-loop approach, where the relation between the input

and output signals is described by the open-loop process model, as shown in Figure 3.

Figure Nº 3. Open-loop FD scheme.



From Figure 3, it can be seen that the FD system can be designed independently of the way as the input signal is generated, i.e. if it is a known external input signal or it comes from a feedback controller. Hence, in theory, the MPC controller not affects the performance of the FD system. But, in practice, this affirmation is not valid. For instance, sensor faults have no influence on the process dynamics, except through a feedback control. Moreover, perfect models do not exist nor there are common characteristic to all possible model uncertainties, which are difficult to deal and whose effects are fed back by the controller. On the other hand, if the controller is more robust then it attenuates the effects of the failure on the plant output. Therefore, in conclusion, feedback controller deteriorates

the performance of the FD system (Sotomayor, 2006).

In this work, we intend to design a FD system that will be able to detect abnormal situations in the polymerization process, namely changes in the process parameters  $A_i$ ,  $f_i$ ,  $M_m$  and disturbances in the temperature  $T_f$ . For this purpose, the FD system requires the use of the detailed phenomenological model of the process than the linear model used in controller design. According Eqs. (1)-(7), the process model can be written in the following nonlinear state-space form:

$$\begin{aligned} \frac{dx(t)}{dt} &= g(x(t), u(t), f(t)) \\ y(t) &= h(x(t)) \end{aligned} \tag{19}$$

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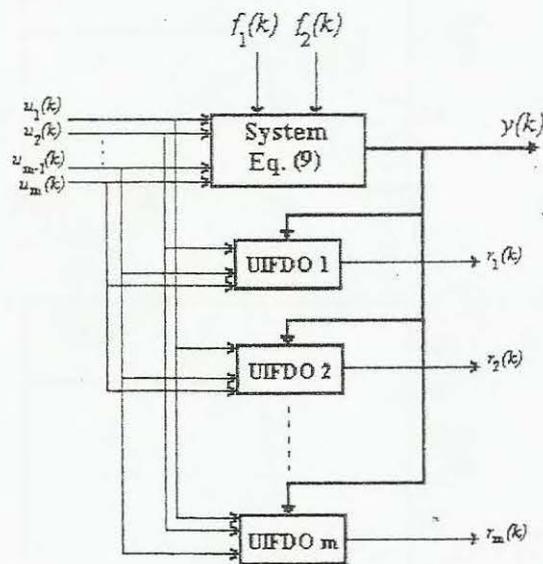
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where:

$\bar{x} = [[I] \ [M] \ T_e \ T_c \ D_0 \ D_1]^T$  is the state vector,  $\bar{u} = [Q_i \ Q_c \ Q_s]^T$  is the input vector,  $\bar{y} = [\eta \ T_e]^T$  is the output vector and  $\bar{f} = [A_i \ f_i \ M_m \ T_f]^T$  is the fault vector. Using a truncated Taylor expansion, this model is linearized, around the operating point  $(\bar{x}_0(t), \bar{u}_0(t), \bar{f}_0(t))$  shown in Tables 1 and 2. The linearized model in deviation form can be described by a discrete system similar to Eq. (9), with a sampling time  $\Delta t$ , where  $x = \bar{x} - \bar{x}_0$ ,  $u = \bar{u} - \bar{u}_0$ ,  $y = \bar{y} - \bar{y}_0$  and  $f = \bar{f} - \bar{f}_0$ .

Based in this linearized model, a bank of four UIFDO is implemented in a generalized observer scheme (GOS) (see Figure 4). This bank of observers produces a generalized residual set, where each residual is supposed to be insensitive to a particular fault and sensitive to all other faults. Of this way it is possible to isolate the fault.

Figure N° 4. A GOS scheme for fault detection and isolation.



Because the nonlinear features of the reactor, and in order to reduce process/model mismatch, we prefer to use observers with adaptive gain, in the form of a Kalman filter, instead of static gain. Therefore, the observer gain  $K$  in Eq. (17) is updated as follows:

$$K(k) = \left( \bar{A}_{22} P(k-1) C_{22}^T \right) \left( I + C_{22} P(k-1) C_{22}^T \right)^{-1} \quad (20)$$

$$P(k) = (\bar{A}_{22} - K(k) C_{22}) P(k-1) \bar{A}_{22}^T \quad (21)$$

where  $P$  is the prediction error covariance matrix. Finally, the residuals are evaluated on a residual evaluation function of the form:

$$J(r(t)) = N(1-\lambda) \sum_{i=0}^{\infty} \lambda^i r(t-i) \quad (22)$$

with a weighting factor  $N = 10$  and exponential forgetting factor  $\lambda = 0.1$ . The fault magnitude is estimated using state  $z_1(k)$  inferred with Eq. (15) and substituting the result into Eq. (11). Therefore, the estimation of the fault is obtained from the insensitive observer as:

$$\hat{f}_1(k) = (E_{11})^+ [z_1(k+1) - A_{11} z_1(k) - A_{12} z_2(k) - B_1 u(k)] \quad (23)$$

It can be seen from Eq. (23) that the estimation of the fault magnitude at instant  $k$  depends on the inferred state  $z_1$  at instant  $k+1$ . To avoid this problem, the computation of the fault estimation is delayed one sampling period. The performance of the FD system is evaluated for two abnormal situations as shown below. For more discussion on this subject see Sotomayor and Odloak (2005).

#### Abnormal situation 1: Change in parameter $A_i$

This fault scenario corresponds to a change in the termination rate constant  $k_t$ , which is the sum of the effects of reaction disproportionation and combination. These contributions are not easily estimated as they vary with temperature and composition, causing an uncertainty in the overall constant  $k_t$ . In addition  $k_t$ , presents a phenomenon known as gel or Trommsdorff effect, when its value falls due to strong diffusion limitations at higher monomer conversions.

In this study, we consider an abrupt decrease of 5% in parameter  $A_t$  occurring at  $t = 50$  h. As can be seen in Figure 5, the fault is isolated perfectly, since it is alarmed by residual  $r_{fi}$ ,  $r_{Mm}$ ,  $r_{Tf}$ , and not by residual  $r_{At}$ . Figure 6 shows the estimation of the fault. The detection and isolation of this fault is achieved in approximately 2 h and their estimation in 15 h, after the fault occurrence.

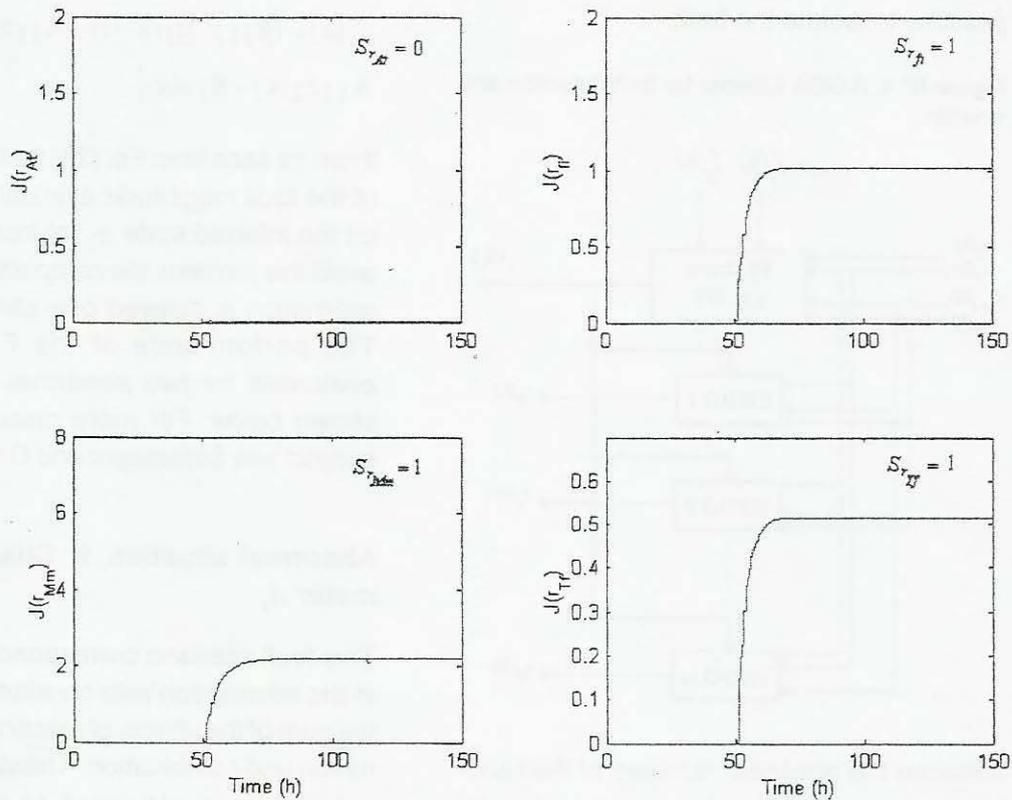
**Abnormal situation 2: disturbance in temperature  $T_f$**

This fault scenario is harmful, since small increase in change in steady-state temperature of reactor results in heat generation exceeding heat removal, which

causes the reactor to operate at the upper steady-state. Likewise, if there is a small decrease in steady-state temperature, heat removal dominates heat generation, causing the reactor to operate at the lower steady-state.

Here, it is simulated a sudden increase of  $0.5^\circ\text{K}$  in the feed temperature  $T_f$ , occurring at  $t = 50$  h. Figure 7 shows that, the residuals  $r_{At}$ ,  $r_{fi}$  and  $r_{Mm}$  are sensitive and residual  $r_{Tf}$  is insensitive to this disturbance. Figure 8 presents the estimation of the disturbance magnitude. For this case, complete detection and isolation is obtained in approximately 2 h and their estimation in 7 h, after the disturbance occurrence.

Figure N° 5. Residual responses for change of 5% step decrease in parameter  $A_t$ .



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Figure N° 6. Estimation of fault in parameter  $A_f$  (-5%).

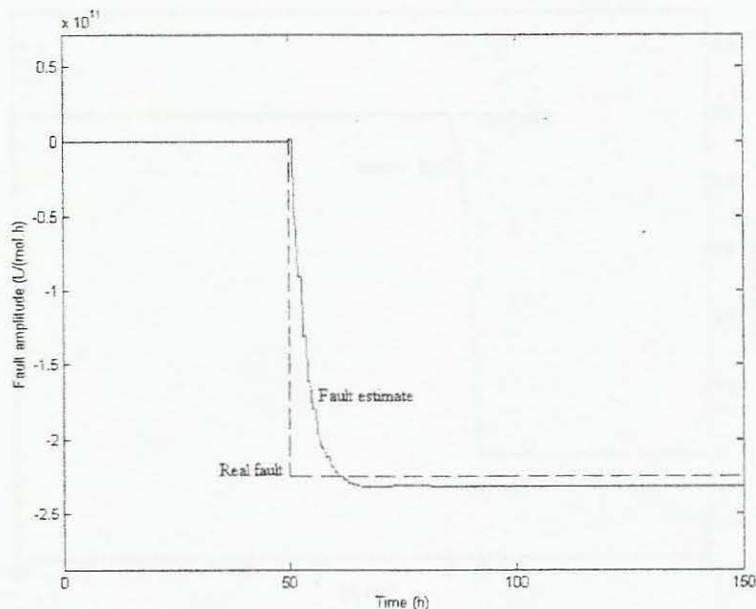


Figure N° 7. Residual responses for disturbance of 0.5°K step increase in temperature  $T_f$ .

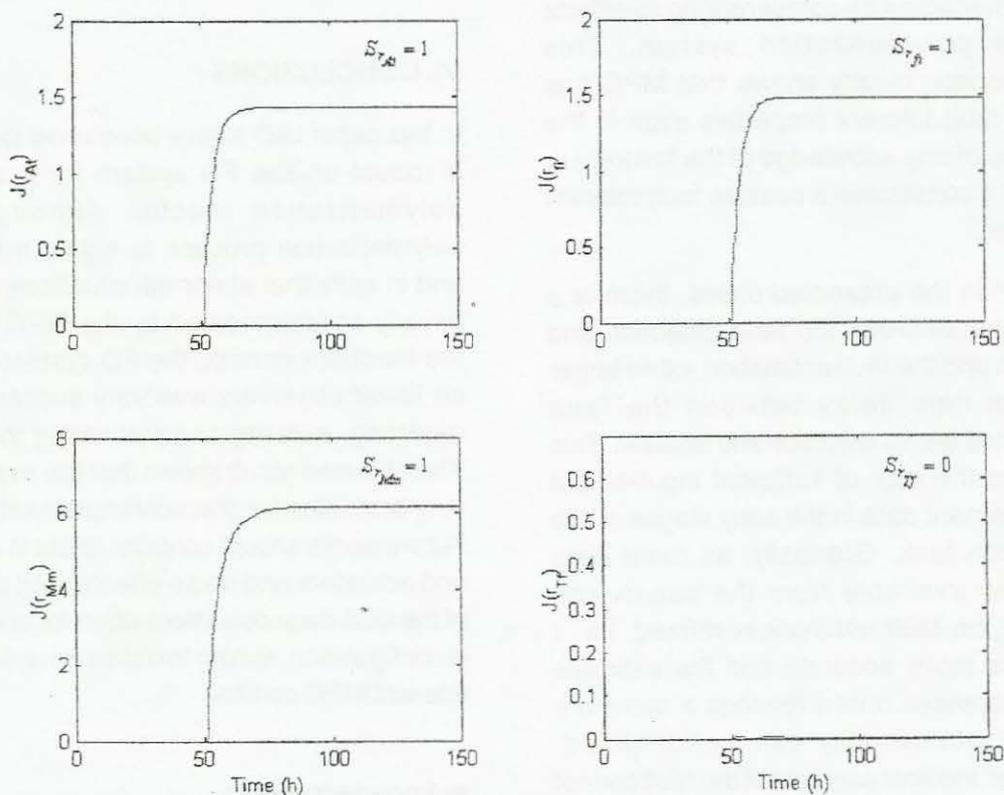
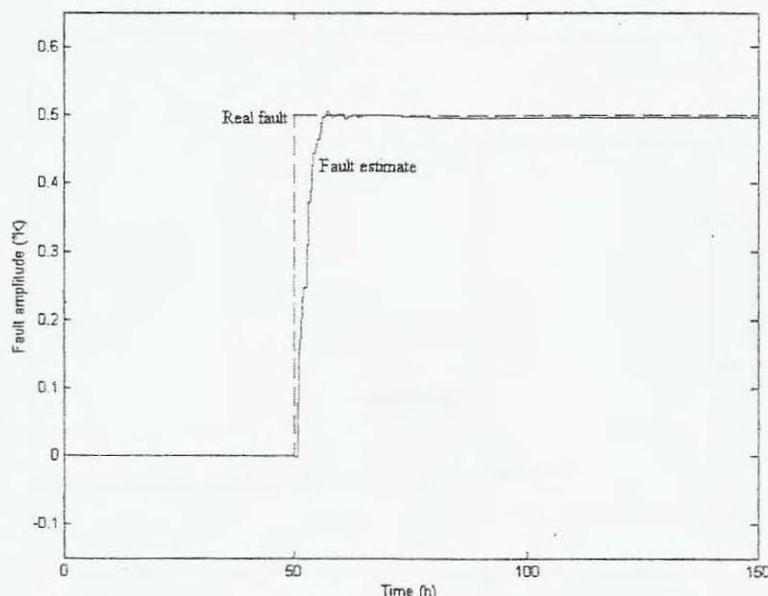


Figure N° 8. Estimation of disturbance in temperature  $T_f$  (+0.5°K).



Although the abnormal situation is actually present, the MPC control system accommodates it by compensating its effects on the polymerization system. This characteristic clearly shows that MPC has certain fault tolerant properties even in the absence of any knowledge of the failure, i.e. by itself it constitutes a passive fault tolerant controller.

As seen in the presented cases, there is a time delay between the fault detection and isolation and the fault estimation, often larger than the time delay between the fault occurrence and its detection and isolation. This is due to the lack of sufficient input-output measurement data in the early stages of the estimation task. Gradually, as more data becomes available from the supervised system, the fault estimate is refined, i.e. it becomes more accurate and the estimate error decreases until it reaches a minimum and the abnormality can be identified. Moreover, the final estimate of the fault cannot be expected to match perfectly the true value of the fault, due to model uncertainties. Therefore, imperfections of the fault diagnosis system, in terms of delays and model

uncertainties, should be taken into account if control reconfiguration is to be considered.

## VI. CONCLUSIONS

In this paper UIO's have been used to design a robust on-line FD system for a styrene polymerization reactor. Although the polymerization process is highly nonlinear and in spite that abnormal situations can be usually accommodated by the MPC due to the feedback control, the FD system based on linear observers was very successful in detecting, isolating and estimating the fault. The obtained result shows that the method is very promising for practical implementations. Future works should consider faults in sensor and actuators and noise effects, and the use of the fault diagnosis information for controller reconfiguration, aiming to obtain an active fault tolerant MPC control.

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VII. REFERENCES

1. Chen, J., R.J. Patton. Robust Model-Based Fault Diagnosis for Dynamic Systems. *Kluwer Academic Publishers*. Norwell, MA., 1999.
2. Embiruçu, M., E.L. Lima, J.C. Pinto. *Polymer Engineering and Science*, 36, 433, 1996.
3. Frank, P.M., X. Ding. *Journal of Process Control*, 7, 403, 1997.
4. Hou, M., P.C. Müller. *International Journal of Control*, 60, 827, 1994.
5. Huang, Y., G.V. Reklaitis, V. Venkatasubramanian. *Industrial and Engineering Chemistry Research*, 41, 3806, 2002.
6. Kaboré, P., S. Othman, T.F. McKenna, H. Hammouri. *International Journal of Control*, 73, 797, 2000.
7. Kumar, V., U. Sundararaj, S.L. Shah, D. Hair, L.J. Vande Griend. *Polymer Reaction Engineering*, 11, 1017, 2003.
8. Maner, B.R., F.J. Doyle, B.A. Ogunnaike, R.K. Pearson. *Automatica*, 32, 1285, 1996.
9. Patton, R.J., J. Chen. *Control Engineering Practice*, 5, 671, 1997
10. Qin, S.J., T.A. Badgwell. *Control Engineering Practice*, 11, 733, 2003.
11. Rodrigues, M.A., D. Odloak. *Automatica*, 39, 569, 2003.
12. Schnelle, P.D., D.L. Rollins. *ISA Transactions*, 36, 281, 1998.
13. Sebzali, Y.M., X.Z. Wang. *Journal of Loss Prevention in the Process Industries*, 15, 555, 2002
14. Sotomayor, O.A.Z. Feedback Control Effects on the Fault Diagnosis Performance. (In Preparation) 2006.
15. Sotomayor, O.A.Z., D. Odloak. *Chemical Engineering Journal*, 112, 93.
16. Tatara, E., A. Cinar. *ISA Transactions*, 41, 255. 2002.

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